Modeling

The Prediction Problem for Salinity Intrusion

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Salinity prediction in an estuary such as Galveston Bay is deceptive: it appears simple, should be solved, and yet, is a continuing source of controversy. On the one hand, salinity is the quintessential estuarine parameter, virtually conservative, and easy to measure, so there should be an extensive data base. Moreover, predictive analyses of salinity have been carried out for about a century. The earliest estuary digital models addressed salinity, and for the Texas estuaries, the state has invested a considerable effort in model development and verification. On the other hand, when issues arise involving salinity intrusion, such as freshwater inflow releases to ameliorate high salinities, or proposed enlargements of a ship channel, the scientific assessments dissolve into dialectics, focusing on the unreliability of salinity prediction.

There are two general techniques: statistical analysis based upon historical measurements; and deterministic modeling. The first relies solely upon the available data base, and seeks to establish relations between salinity and the controlling variables. There are two problems. First, the relations are difficult to extract. Second, any change in the physical system must be discriminated in the data base, and may invalidate the empirical basis of the statistical relations.

The universal choice for independent variable is freshwater inflow. Probably no analysis has provoked as much frustration in estuarine water quality because there is a clear, intuitive cause-and-effect association of salinity with freshwater inflow that refuses to emerge from the statistics (e.g., TDWR, 1981). Salinity in an embayment such as Galveston Bay *is* dependent upon freshwater inflow. Without freshwater inflow to the bay, the salinities would eventually acquire oceanic values. The fallacy is to conclude from this that there is a *direct* association between a given level of inflow and the salinity at a point in the bay. Other hydrographic mechanisms, such as tides, meteorology, and density currents, as well as the boundary value in the Gulf of Mexico, govern the internal transports of waters of different salinities in the bay, and dictate how freshwater influences salinity.

The nature of the problem is illustrated by the salinity data of Fig. 1, showing the association of mid-bay salinities with gauged flow of the Trinity. While there is a discernible downward slope in the relation, as we would expect, the variance of salinity encompasses nearly the entire estuarine range, independent of the level of inflow. This high variance is a quantitative demonstration of the complexity of the response of salinity in the bay to many factors, only one of which is freshwater inflow. Even if the freshwater-inflow signal is optimally pre-averaged, to minimize

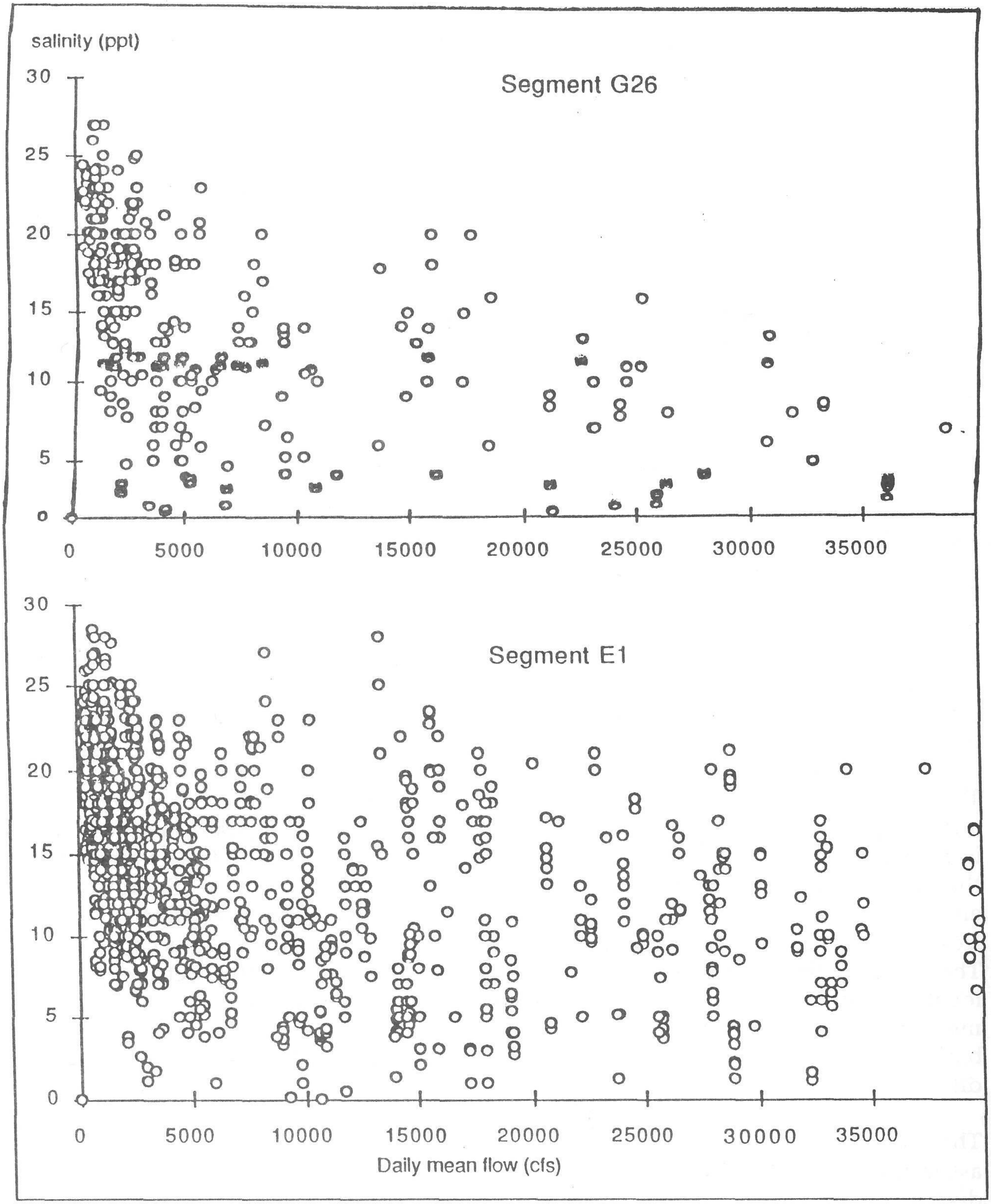

Figure 1. Salinity (upper 1.5 m) in mid-bay segments versus Trinity River flows, for two hydrographic segments. Data are from Ward and Armstrong (1992).

the standard error of the regression, the explained variance is little better than 50%, and even worse in areas of the lower bay. Further, the standard error of the regression is still more than 4 ppt, which means the regression predicts salinity at a 95% certainty within a 16 ppt range, i.e., about half the normal range from fresh to oceanic. This is not sufficiently precise for most management requirements.

The second problem of violating the empirical basis of the data is demonstrated by the problem of a proposed channel enlargement. If we had a suitable statistical relation between salinity and inflow, say, the data would reflect the present dimensions of the channel. The same relation could not be expected to work with enlarged channel dimensions and, therefore, could not be used as a predictor. The only means of predicting the effect of a channel on salinity by statistical analysis would be to employ channel dimensions as an independent variable in the analysis. But channels are usually enlarged incrementally over a long period of time. In Galveston Bay, the trans-bay reach of the Houston Ship Channel evolved as follows (depth in feet and completion date): 12 in 1880; 19 in 1910; 25 in 1914; 30 in 1922; 32 in 1937; 36 in 1950; and 40 in 1965. Thus, to find salinity data for even a 10% change in channel depth would require data from the 1950-65 period. Earlier than this, salinity data is virtually nonexistent. Moreover, to extract the effect of a 10% change in channel dimension from all of the other sources of variance (such as river impoundment) underway during the same period may be impossible. (In one instance on the Texas coast, a deep-draft channel was dredged through a bay without any previous channelization, *viz.* the 36-ft ship channel in Matagorda Bay, dredged in 1963. Pre-channel and post-channel salinities were analyzed by Ward (1983) to determine a systematic increase of about 5%.)

The second general predictive technique, deterministic modeling, should in principle incorporate all of the relevant physical processes and, therefore, permit evaluation of modified inflow levels, altered channel dimensions and other changes. And here there are two problems. First, some features, such as ship channels or barriers to flow, have an influence on salinity far in excess of their spatial dimensions, so the model must be able to resolve these features. Second, and more importantly, the physical processes governing salinity intrusion are especially difficult to model.

Typical dimensions of the width of a dike or a ship channel are a few hundred meters, compared to the typical dimension of an embayment of several tens of kilometers. The spatial resolution of a numerical grid may be as small as 1 km, which for various reasons is about the limit of computational feasibility for practical computers, but this is still an order of magnitude larger than the channel. The present solution to the resolution problem is to use variable-scale numerical grids. These include: (1) finite-elements which conform to the physical feature; (2) boundary-fitting orthogonal grids, which accomplish the same thing in a finite-difference framework; (3) transformed coordinates that expand the scale of resolution; and (4) nested grids, i.e., finer-resolution networks embedded within critical areas of the system. Fig. 2 shows an example of resolution of a channel in an

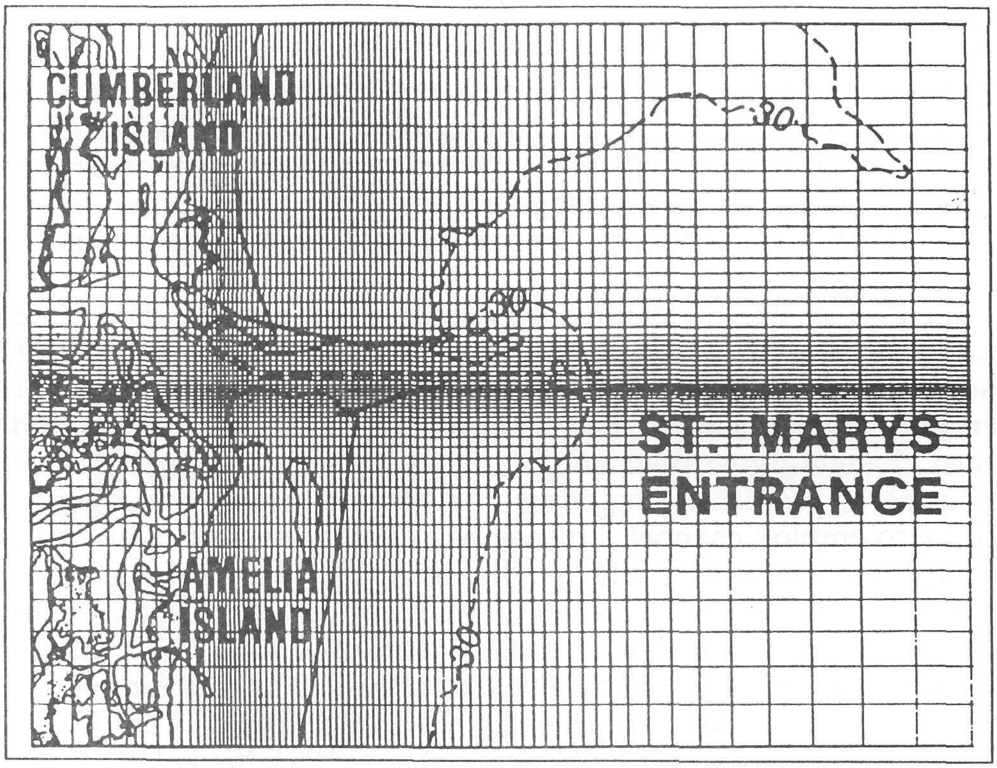

Figure 2a. Transformed coordinate resolution of inlet to King's Bay (Vemulakonda, et al., 1988)

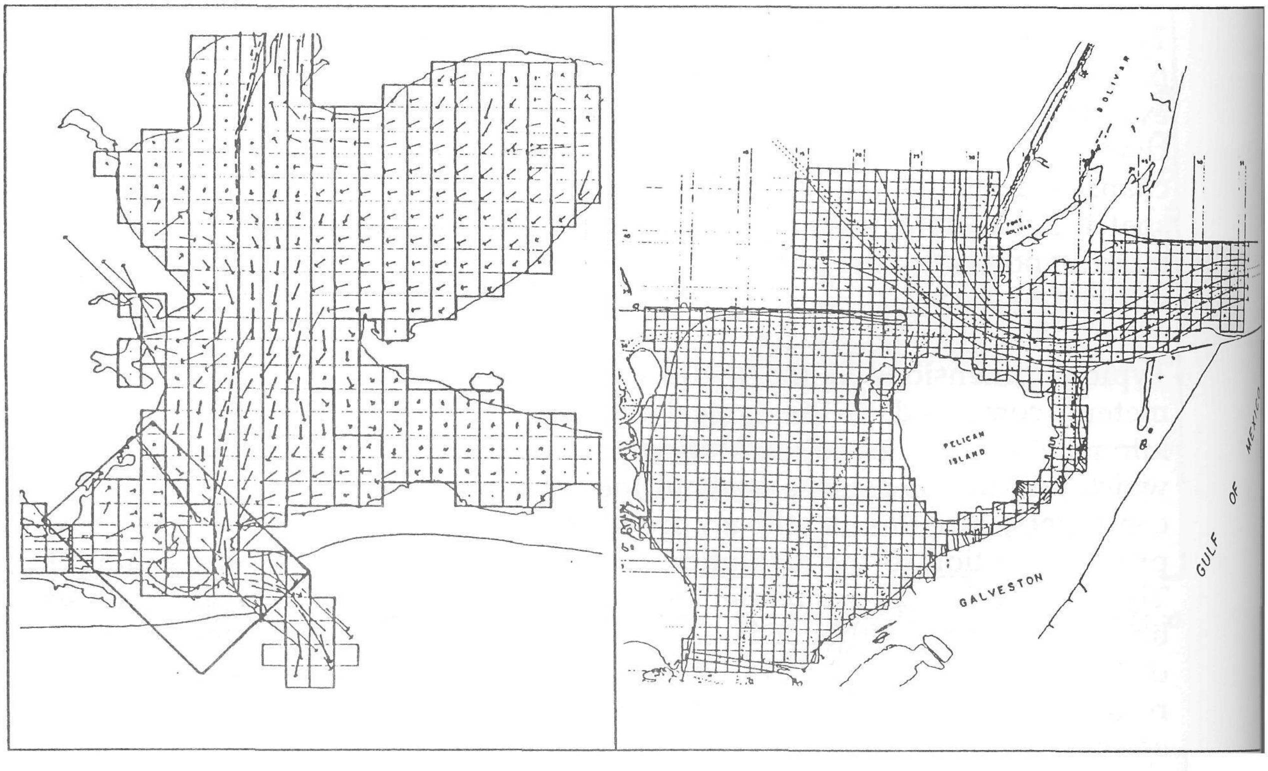

Figure 2b. Nested grid resolution of inlet to Galveston Bay (Espey, Huston & Associates, 1979).

estuary using transformed coordinates, in this case St. Mary's Entrance to Kings Bay, and of nesting a fine-resolution mesh in a coarser grid, for the inlet vicinity of Galveston Bay. Each of these strategies imposes computational problems of stability and accuracy (as well as economics), but they are in principle a workable solution, provided the basic model is adequate.

The greater problem is proper depiction of the physical processes of salinity intrusion in the model. As noted in the introduction, salinity is virtually conservative so its modeling hinges on transport processes. This is a source of paradox in estuary modeling, that salinity has been modeled for decades, but cannot be reliably predicted: its historical role in modeling has been a "calibrator" for mathematical formulations of (highly averaged) transport, e.g., the "mixing matrix" of the Thames model (WPRL, 1964, see also Ward and Espey, 1971) or the familiar one-dimensional steady-state analysis (Harleman, 1971). Only since the 1960s has numerical modeling sought to attack the hydrodynamic processes directly, motivated by the need to better treat geometrical complexity than possible with longitudinal-type models. In these models, salinity is treated as a passive tracer and modeled by a feed-forward process of first determining the currents given tides and inflows, then computing the salinity distribution, see Fig. 3.

Unfortunately, salinity governs density, and density exerts a major control on hydrodynamics, so currents cannot be determined independently of salinity. One important manifestation of this is the estuarine density current, which produces a net counterflowing circulation in deep, narrow systems (upstream transport in the lower layer) and net horizontal circulations in shallow systems (upstream transport along the axis of greatest depth). Because the intensity of density currents increases roughly as the cube of depth (Ward, 1983), the process is extremely sensitive to depth and is one of the prime mechanisms for preferential salinity intrusion in a deep channel.

A feedforward model as displayed in Fig. 3 cannot predict such a transport. In order to get the transport of salinity correct in such a model, a "dispersion" term is added to the salt balance equation. There is no theoretical basis for such a term, and no *a priori* means of computing it. The dispersion coefficients, rather, are set to those values necessary to replicate observed salinity distributions. Once again, salinity

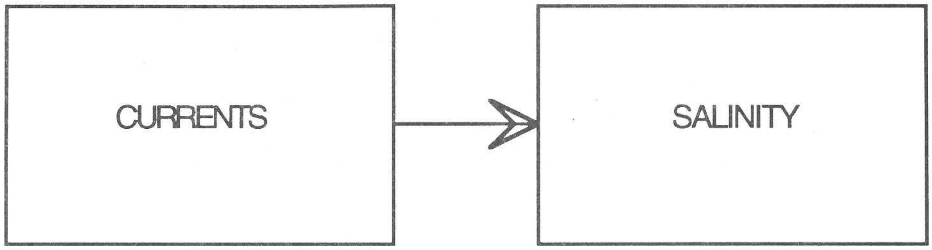

Figure 3. Feedforward model of salinity.

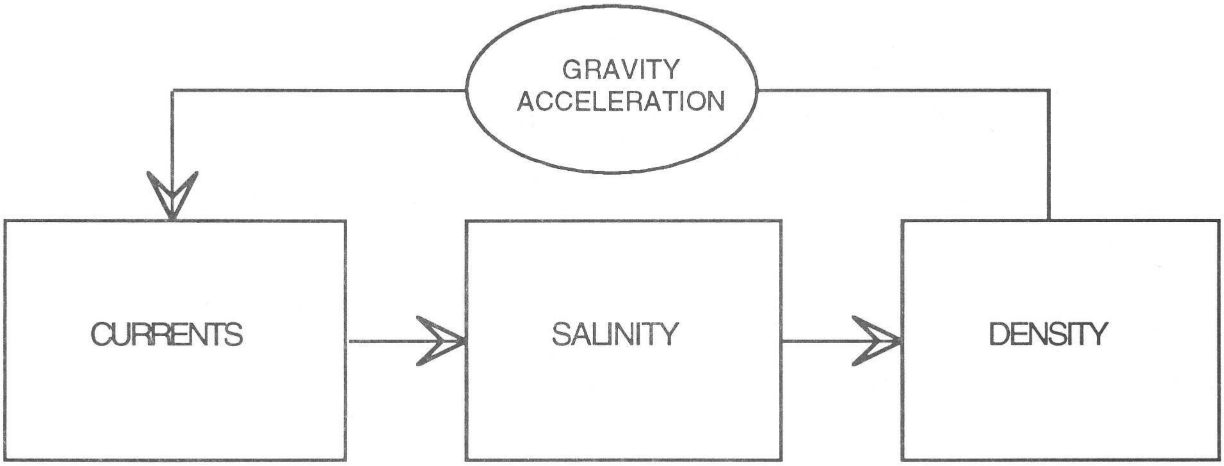

Figure 4. Coupled hydrodynamic/salinity model with feedback for density currents.

becomes a calibrator for hydrodynamics. This is the formulation used by the TWDB bay models in the early 1980 inflow reports (e.g., TDWR, 1981) and by the present version of DYNHYD, the hydrodynamic module of EPA's WASP. At best, such a model should be regarded as a means for extrapolating salinity beyond the configuration used for calibration.

The correct approach is to couple hydrodynamics and salinity, through the density term, as indicated in Fig. 4. This is analogous to Fig. 3, except a feedback loop is added to suggest the coupled calculation. This is a nontrivial alteration. It requires simultaneous storage of the hydrodynamic variables and salinity and, therefore, greater computer demands. More importantly, advective transport of salinity becomes nonlinear, which opens the door to numerical difficulties as well as pathological mathematical behavior. The more recent versions of the TWDB bay models, which employ a finite-element technique, incorporate the coupled solution of currents and salinity.

But there is an another, more subtle aspect to the effect of salinity on hydrodynamics. This is the influence of vertical density gradients on the intensity of turbulence. Vertical turbulent fluxes control the dissipation of momentum by bed friction, the acceleration of the water column by surface stresses, and the rate of salinity intrusion due to its vertical flux. A vertical density gradient creates a dissipation of turbulent energy in working against gravity. The distribution of salinity is dictated in part by the adjustment of its own vertical stratification to the sources of turbulent energy seeking to de-stratify it. Even if salinity is unstratified, it has exerted an effect on the vertical turbulent fluxes.

The more complete hydrodynamic-salinity model takes the form of Fig. 5, with salinity feedback in both the gravitational terms and the turbulent terms. All of the above-noted problems of nonlinear coupling are still present. Now there is an additional feedback loop with *additional* nonlinear coupling. Moreover, we do not

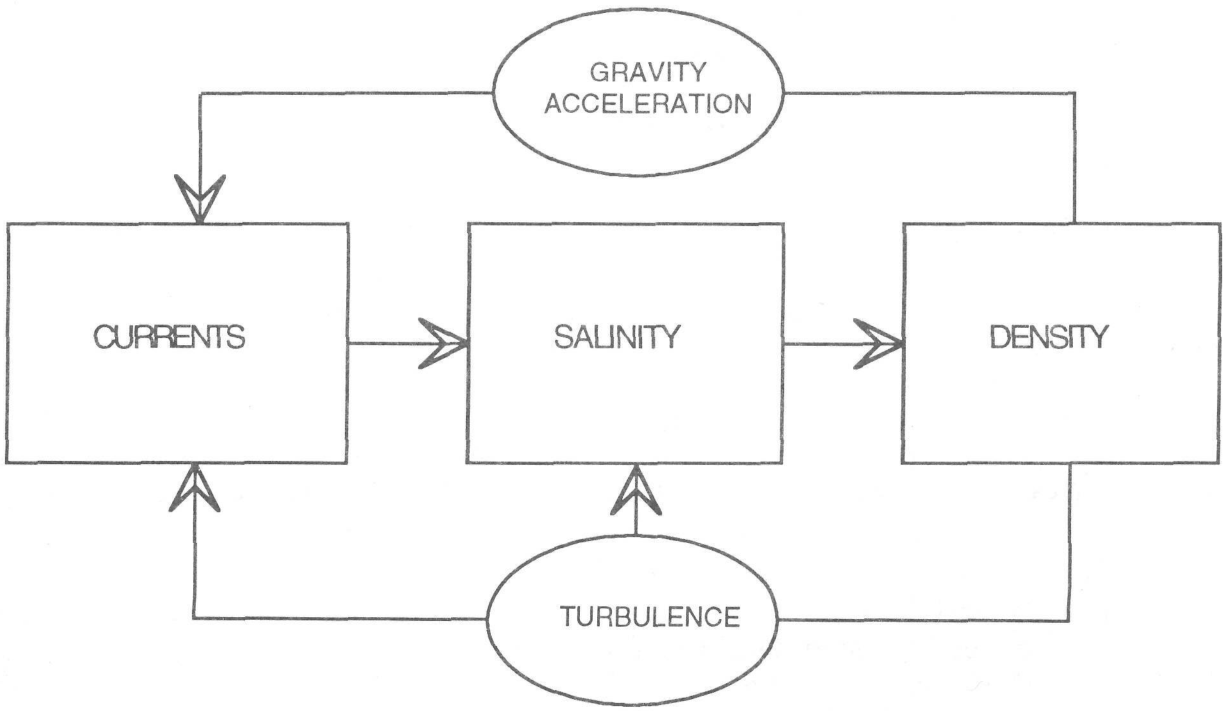

Figure 5. Coupled hydrodynamic/salinity model with feedback for density currents and turbulent fluxes.

have an adequate formulation for the turbulent processes. And, further, explicit depiction of the vertical coordinate appears necessary, even for a bay which is substantially well-mixed in the vertical. The inclusion of the vertical coordinate in turn increases the computational demands of the model several-fold just to accommodate the additional points of calculation, and requires much greater care in the expression of boundary terms at the surface and bottom.

Modeling of turbulent fluxes in a density-stratified fluid is especially problematic. Analysis of field data and heuristic reasoning suggest the eddy flux should be an inverse function of Richardson number (e.g., Kent and Pritchard, 1959) or Brunt-Väisällä frequency (Ward, 1977). However, the mathematics are improperly closed and the use of this formulation in a numerical model leads to a type of instability that must be controlled by strictly bounding the value of the eddy coefficient, which amounts to the same thing as *a priori* prescribing its value. More promising is the use of higher-order closures, e.g., Mellor and Yamada (1982), which is the basis for the Princeton estuary model (Oey et al., 1985).

A recent review listed 11 numerical hydrodynamic models potentially applicable to Galveston Bay (Ward, 1991) of which most require a mainframe computer or even a parallel processor. Certainly, inclusion of the vertical coordinate is one of the major reasons for such computer demands. Yet, many estuaries such as Galveston Bay are, at least on the large scale, practically two-dimensional. Some *rational* means of parameterizing the nonlinear density-coupling of Fig. 5 is needed to enable treatment of the system as two-dimensional.

Even if we have analyzed and incorporated all of the relevant physical processes — either statistically or deterministically — and formulated the model in some efficient, realizable way for a system like Galveston Bay, there is still remaining a major philosophical problem of salinity prediction. This is that we have not yet come to grips with the nature of salinity as a time signal. Consider again Figure 1 plotting the dependence of salinity upon inflow, and explore the reasons for the high variance.

There are several scales of time variation in the salinity signal, ranging from short-term tidal and meteorological to long-term seasonal and multi-yearly. A recent analysis of salinity in the Texas bays by the National Ocean Service seeks to better quantify this variability and the factors which force variability. The summary matrix for Galveston Bay is shown in Fig. 6. Any single measurement of salinity is potentially influenced by all of these time scales. At the outset, we commented that there should be an extensive data base for salinity. For Galveston Bay, the Status & Trends project (Ward and Armstrong, 1992) compiled about 77,000 independent measurements of salinity (using all available proxy measures, including conductivity, light refraction, chlorides, and density). Since then, perhaps another 20,000 have come to light, so we have about 100,000, mainly since 1960. If these are uniform in time (which they are not), and uniform in space, distributed into about 50 hydrographically distinct areas of Galveston Bay (which they are not), this gives about 60 per year per area. Therefore, the data base is inadequate to resolve time scales of less than about a week. The tidal variability, for instance, is virtually unsampled in Galveston Bay (as indicated in Fig. 6). Thus, the data of Fig. 1 includes random sampling of these shorter time scales, which is nonresolvable and an intrinsic source of variance.

MECHANISM	TIME SCALE				
	Hours	Days	Weeks	Months to seasons	Year to year
Freshwater inflow			M (freshet)	D (seasonal discharge)	D (wet/dry)
Tides					
Wind		S (frontal passages)			
Other: Channels			M (density currents)	S (density currents)	
Shelf river plumes				S	M

D: Dominant factor accounting for the greatest range in salinity variability
S: Secondary factor having an influence on salinity variability
M: Minor factor having a detectable influence on salinity variability

Figure 6 Time variability and controls for salinity in Galveston Bay, from Orlando et al. (1991)

A second source of variance is due to the response *per se* of salinity. Take the response to freshwater inflow as an example. First, there is a lag between the freshwater signal as measured at an inflow gauge and its effect on the bay. In addition to this lag, salinity in the bay responds more as an integrator of freshwater inflow, i.e., with a longer time scale of variation than that of the inflow itself. Moreover, the response of salinity is affected by the operative physical processes, e.g., tidal excursion, antecedent salinity gradients, semi-permanent circulation patterns. Salinity *intrusion* takes place by mixing by tidal currents and advection by density currents, and intrusion into the upper bay generally requires a long time, on the order of weeks to months. Salinity *extrusion*, especially in Trinity Bay and upper Galveston Bay, on the other hand, is basically a mechanism of displacement by freshwater, and occurs rather rapidly when forced by freshets. It is not surprising, therefore, that there is no unique relation between salinity and inflow, but rather a range of responses, which are not separated in analyses like Fig. 1.

Even in posing management questions, we do not confront the time signal nature of salinity. Evaluations of freshwater inflow on salinity or physical modifications invariably treat average salinity, usually some sort of statistical steady state. The biological impacts are probably not governed by long-term averages, but rather duration and magnitude of extremes, e.g., low salinities during spring, high salinities during summer. Asking the right question is half of the prediction problem.

Acknowledgments

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3-D Hydrodynamic Model of Galveston Bay

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The U.S. Army Engineer Waterways Experiment Station (WES) Hydraulics Laboratory (HL) has developed a three-dimensional (3D) hydrodynamic model of Galveston Bay for the Houston-Galveston Navigation channels, Texas project, in cooperation with the U. S. Army Engineer District, Galveston. The model used is RMA10-WES, which is one of a suite of models known collectively as the TABS-MD system. The 3D model is capable of computing water velocity, circulation patterns, salinity gradients, and water levels for the entire Bay system.

The model uses Finite Element formulation, which allows incorporation of complex geometric features. The model consists of a network or mesh of computational nodes defined as x, y, and z coordinates. These nodes are then tied together to form elements, which may be assigned properties that reflect actual conditions of Bay, such as roughness of the bed and eddy viscosities of the water. The model is driven by imposing values for salinity at each node and values of forcing functions at the boundaries. These consist of a tidal variation in the Gulf of Mexico, freshwater inflow at sixteen points around the Bay, Gulf salinities, and wind speed and direction. These values are varied through time in increments from 15 minutes to one hour, termed time steps. By applying actual observed or hypothetical values, such as variations in freshwater inflow at the boundary, the effects of these can be observed and/or predicted at each computational point in the mesh. The Galveston Bay model consists of approximately 12,000 computational nodes, which form 5,100 elements.

The model has been used to evaluate existing Bay conditions and several geometries based on proposed channel enlargement plans. The existing condition consists of the Bay with a nominal 40 foot deep and 400 foot wide Houston Ship channel. The Phase I plan features a 45 foot deep channel and a 530 foot wide channel. The Phase II plan features a 50 foot deep channel that is 600 feet wide. The Phase I and II plans also included some 18 sites where the material excavated from the channel would be put to beneficial uses such as creation of marsh, bird, and boater destination islands. Additionally, a National Economic Development (NED) Plan was run that evaluated open bay disposal of the excavated material over a portion of the bay next to the Houston Ship Channel.

The model has been used not only to evaluate several geometries but also several hydrological scenarios of water use in the Houston area. These hydrologic scenarios were based on construction of the Wallisville dam on the Trinity River and shifts in use of surface and groundwater through the year 2049. The model runs were of two durations. One series of tests was one year long, January through December. These were termed X class runs. Another series of tests was nine months long and was

Figure 1. Existing conditions. July average salinity and medium freshwater inflow. Top and bottom layers are represented by darker isohalines.

Figure 2. Phase I conditions. July average salinity and medium freshwater inflow. Top and bottom layers are represented by darker isohalines.

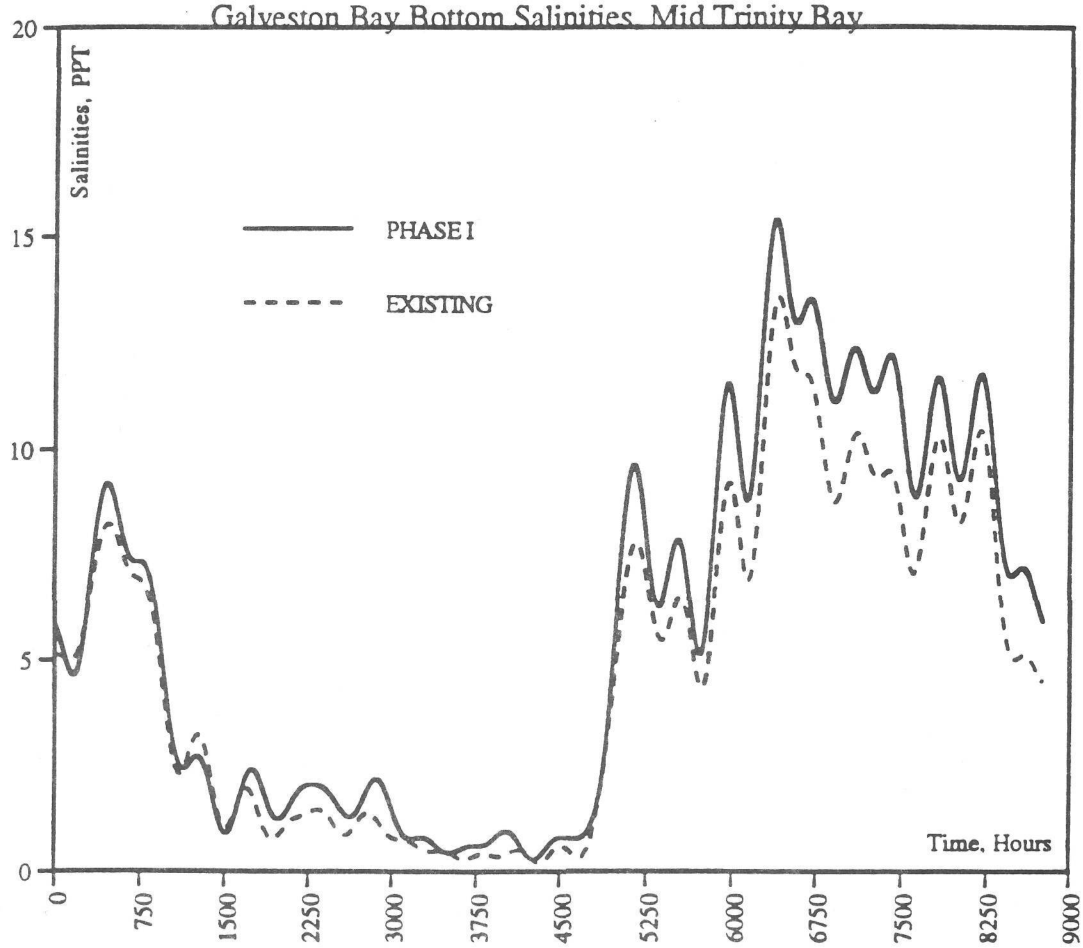

Figure 3. Salinity concentrations (parts per thousand) versus time (hours). Existing and Phase I conditions in mid-Trinity Bay.

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Modeling Toxic Materials in Galveston Bay

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Need for Study

The history of pollution in Galveston Bay is closely tied to the development of urban areas, primarily the City of Houston and associated industries, and other cities and industries of the Bay's periphery. Water quality problems from biodegradable organic wastes peaked in the early 1970s, then decreased with improved waste treatment. The exact status of toxic materials in the Bay is still unknown, however, for there have been few definitive studies to delineate toxic material concentrations. Armstrong (1980) summarized the knowledge of toxic materials in Galveston Bay based on toxic material discharges, toxic material concentrations in the Bay, and an algal assay used to detect growth rate depression due to toxic materials. Armstrong used information from the original Galveston Bay project (e.g., Beal, 1975; Oppenheimer et al., 1973) and concluded that specific toxic materials were present in concentrations believed to affect organisms in the Bay. Estimates of the discharge of toxic materials to Galveston Bay by Neleigh (1974) and Goodman (1989) determined that a variety of toxic materials were being discharged to Galveston Bay from point sources and tributaries.

The current Galveston Bay National Estuarine Program (GBNEP) has several projects underway which are providing toxic material loading data (Armstrong and Ward, 1991) and concentrations of toxic materials in Bay water and sediments (Ward and Armstrong, 1991). There will also be attempts to qualitatively relate loadings to in-Bay concentrations. This can be done to some extent by juxtaposing loading locations to spatial distributions of in-Bay concentrations, but a more effective procedure is to use a mass-balance based mathematical model. The only attempt known to the authors to model toxic materials in Galveston Bay was the work of Ward with Copeland and Fruh (1970) in which the algal growth suppressant was modeled as a conservative material using the Texas Water Quality Board's two-dimensional transport model for Galveston Bay with one-nautical mile square grid. While this attempt appeared to be relatively successful, no successive attempts have been performed on the growth suppressant or specific toxic substances.

By combining the enormous data base that will be available at the end of the above GBNEP studies for loadings of toxic materials from point and nonpoint sources, the analysis of toxic materials in Bay water and sediments, and general knowledge of hydrography of Galveston Bay from earlier studies, it should now be possible to establish cause and effect relationships between discharges and bay concentrations to support the GBNEP objectives.

Objectives

1. To apply the US EPA model TOXI4 to Galveston Bay using the two and three dimensional features of the model for four generic and several selected specific organic materials;

2. To modify the code of TOXI4 for application to heavy metals and to apply the modified program to heavy metals in Galveston Bay; and

3. To determine the consequences to Galveston Bay of present and altered (both increased and decreased) loadings of toxic materials.

Summary of Work

An existing mathematical model for toxic materials supported by the US EPA through its Center for Exposure Assessment Modeling (CEAM) in Athens, Georgia, is being used in this study. This model is TOXI4, a derivative of the WASP4 model which has been in existence in other forms for almost 20 years and has been used to simulate toxic materials in the Hudson Bay River estuary, James River estuary, Chesapeake Bay, and the Great Lakes in one, two, and three dimensions in steady-state and dynamic modes. The principal work of the project is to apply TOXI4 to toxic materials in Galveston Bay in its present form and a slightly modified form. In its present form, TOXI4 is suited for hydrophobic organic materials at low concentrations (Ambrose et al., 1988). It can be used in a limited fashion for heavy metals, but needs to be modified further if it is to be applied to heavy metals in a serious fashion. The modifications needed include allowing for various complexes of the soluble forms of the metals with organic and inorganic ligands and taking precipitation into account. Such changes need to be made in the code of the WASPB subroutine in the WASP4 model. It is this subroutine for toxic materials which makes TOXI4 a unique WASP4 program (separate, for example, from its sister program EUTRO4 for eutrophication problems).

The Water Quality Analysis Simulation Program-4 (WASP4) was developed by researchers at Manhattan College in New York in the early 1980s. WASP4 helps users interpret and predict water quality responses to natural phenomena and man-made pollution for various pollution management decisions. WASP4 is a dynamic compartment modeling program for aquatic systems, including both the water column and the underlying sediment. The time varying processes of advection, dispersion, point and nonpoint mass loading, and boundary exchanges are represented in the basic *program.*

The WASP4 system consists of two stand-alone computer programs, DYNHYD4 and WASP4, that can be run in conjunction or separately. Because DYNHYD is limited to linear estuaries or rivers, it will not be used in this study of Galveston Bay. WASP4 simulates the movement and interaction of pollutants within the water and is supplied with two kinetic sub-models to simulate two of the major classes of water quality problems: conventional pollution (involving dissolved oxygen, biochemical oxygen demand, nutrients, and eutrophication) and toxic pollution (involving organic chemicals, metals, and sediment). The linkage of either sub-model with the WASP4 program gives the models EUTRO4 and TOXI4, respectively.

The basic principle of WASP4 is conservation of mass. The water volume and water-quality constituent masses being studied are tracked and accounted for over time and space using a series of mass balancing equations. WASP4 traces each water quality constituent from the point of spatial and temporal input to its final point of export, conserving mass in space and time. The mass balance equation for dissolved constituents as used in the program is a three dimensional differential mass balance equation around an infinitesimally small fluid volume. By expanding the small volume into larger adjoining "segments", and by specifying proper transport, loading, and transformation parameters, WASP implements a finite-difference form of the three dimensional equation. For brevity, a one-dimensional equation is given here assuming vertical and lateral homogeneity as:

$$\frac{\partial}{\partial t}(A\,C) = \frac{\partial}{\partial x}\left(-\,U_x\,A\,C \;+\; E_x\,A\frac{\partial C}{\partial x}\right) \;+\; A\,(S_L + S_B) + A\,S_K$$

where:

C	= concentration of the water quality constituent, mg/L
t	= time, days
U_x	= longitudinal advective velocity, m/d
E_x	= longitudinal diffusion coefficients, m^2/d
S_L	= direct and diffuse loading rate, g/m^3-d
S_B	= boundary loading rate (including upstream, downstream, benthic, and atmospheric), g/m^3-d
S_K	= total kinetic transformation rate; positive is source, negative is sink, g/m^3-d
A	= cross-sectional area, m^2.

This equation represents the three major classes of water quality processes — transport (term 1), loading (term 2), and transformation (term 3).

The model network is a set of expanded segments that together represent the physical configuration of the water body being modeled. The network may subdivide the water body laterally and vertically as well as longitudinally. Concentrations of water quality constituents are calculated within each segment, and transport rates of water quality constituents are calculated across the interface of adjoining segments.

TOXI4 is a dynamic compartment model of the transport and fate of organic chemicals and metals in all types of aquatic systems. It combines the transport capabilities described above for WASP4, with sediment and chemical transformation capabilities adopted from the model EXAMS to produce the capabilities described here. Transformation processes included in TOXI4 include: acid-base equilibria; hydrolysis; adsorption-desorption; biodegradation; sedimentation; oxidation-reduction; and photolysis. It simulates the transport and transformation of one to three chemicals and one to three types of particulate material. The three chemicals may be independent, such as congeners of PCB, or they may be linked with reaction yields, such as a parent compound-daughter product sequence. Each chemical exists as a neutral compound and up to four ionic species. The neutral and ionic species can exist in five phases: dissolved; sorbed to dissolved organic carbon (DOC); and sorbed to each of the up to three types of solids. Local equilibrium is assumed so that the distribution of the chemical between each of the species and phases is defined by distribution or partition coefficients. In this fashion, the concentration of any specie in any phase can be calculated from the total chemical concentration.

In an aquatic environment, a toxic chemical may be transferred between phases and may be degraded by any number of chemical and biological processes. Transfer processes defined in the model include sorption, ionization, and volatilization. Defined transformation processes include biodegradation, hydrolysis, photolysis, and chemical oxidation. Sorption and ionization are treated as equilibrium reactions. All other processes are described by rate equations which may be quantified by first-order constants or by second-order chemical-specific constants and environment-specific parameters that may vary in space and time.

TOXI4 uses the finite-difference version of the three-dimensional form of the equation given above to calculate sediment and chemical mass and concentrations for every segment in a specialized network that may include surface water, underlying water, surface bed, and underlying bed. In a simulation, sediment is treated as a conservative constituent that is advected and dispersed among water segments, that settles to and erodes from benthic segments, and that moves between benthic segments through net sedimentation, erosion, or bed load. TOXI4 contains a highly sophisticated multi-layer representation of sediment processes including settling and scour in the upper active layer, bioturbation in that layer, sedimentation to a permanent sediment layer, and bed transport. In the water column, solids transport through advective and dispersive processes is also included. Representation of different types of sediment and/or different sediment sizes linked selectively to transport processes and/or settling rates is possible, also.

In a simulation, the chemical can undergo several physical or chemical transformations. Fast reactions are handled with the assumption of local equilibrium while slow reactions are assumed to follow first order kinetics using a lumped rate constant specified by the user or calculated internally based on summation of several process rates, some of which are second order. The effective first order decay rate can vary with time and space and is recalculated as often as necessary throughout a simulation. The chemical is advected and dispersed among water segments and exchanged with surficial benthic segments by dispersive mixing. Sorbed chemical settles through water column segments and deposits to or erodes from surficial benthic segments. Within the bed, dissolved chemical migrates downward or upward through percolation and pore water diffusion. Sorbed chemical migrates downward or upward through net sedimentation or erosion. Both rate constants and equilibrium coefficients must be estimated in most toxic chemical studies.

Depending on the complexity level one uses with TOXI4, some 18, 30, or 42 kinetic display variables are output for each segment included in the model network and at the printing time steps specified by the user. For one chemical modeled, for example, the concentrations of solids are given (total concentration and concentrations for each of the three types of sediments), the chemical concentrations are given (total concentration and the forms in the dissolved state, sorbed onto DOC, sorbed onto sediments, and in the ionic form), temperature, and the rates for the following transformation processes: biodegradation, hydrolysis, photolysis, volatilization, and oxidation. The dump file into which values for these variables are placed may be manipulated by a post-processor program supplied with WASP4 to extract selected values for variables, segments, and times desired, placed into a table, and imported into spreadsheet programs for further manipulation such as graphing.

In this study, four generic classes of compounds were selected first based on rate of degradation (0 for conservative and > 0 for nonconservative) and partition coefficient (values in the range of 10^2 L/kg and 10^5 L/kg) of compounds found in Galveston Bay, then compounds representing each of these four classes will be selected. The selection criteria to be used are: (1) the compound is present in point source and/or nonpoint source discharges (over 50 organics and metals are now reported by discharges as part of self-reporting requirements); (2) the compound is present in the water and/or sediment in Galveston Bay; (3) the compound is present at a concentration range that is of concern (some metals have already been identified as being of concern and the GBNEP work should identify others as well as organics); and (4) the compound is distinguishable by partition coefficients and transformation rates.

Transport processes information can be obtained from the existing TWC two-dimensional transport model for Galveston Bay, but newer alternatives should be available by the start of this project, namely the COMPAS model for Galveston Bay, or the application of the U.S. Army Corps of Engineers three-dimensional model RMA-10, and/or the three-dimensional Sheng model (CHB-4) developed for Chesapeake Bay and now being coupled with WASP4 (and hence TOXI4) by CEAM.

Specific technical tasks being performed in the study are:

1. Determine the appropriate spatial and vertical segmentation for Galveston Bay based on water and sediment quality data gathered during the analysis of historic water quality data as part of the GBNEP (the segments do not all have to be the same size);

2. Use four generic organic compounds based on rate of degradation, K, (0 for conservative and >0 for nonconservative) and partition coefficient, ¶, (values in the range of 10^2 L/kg and 10^5 L/kg will be used) based on the compounds found in Galveston Bay and other information necessary for modeling these materials with TOXI4;

3. Incorporate necessary modifications to the kinetics of the WASPB subroutine within TOXI4 to be able to model heavy metals;

4. Use the loading estimates of toxic materials from point and nonpoint sources from the GBNEP study (done by the PIs and others), as well as the data from other loading estimates to generate loading inputs to the models, as well as boundary conditions and necessary time functions;

5. Calibrate the models to specific concentrations of toxic organics falling in one or more of the four generic compound categories and to heavy metals;

6. Calculate concentrations of generic and specific organic toxic materials and heavy metals as appropriate in the water and sediment of Galveston Bay using existing and altered loading estimates of these materials; and

7. Find the problem areas of toxic materials within Galveston Bay by comparing water and sediment concentrations to existing US EPA water quality criteria and proposed US EPA sediment quality criteria, and relating the concentrations to the living resources data acquired during the GBNEP study.

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Coupled Oyster-Hydrodynamic Model for Galveston Bay and the Galveston Bay Ship Channel Project

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Galveston Bay is the most important producer of oysters in Texas, typically accounting for 50-80% of the entire Texas fishery. A project designed to widen and deepen the Galveston-Houston Navigational Channel has been proposed.

The channelization project potentially could impact the oyster populations of Galveston Bay in two ways:

(1) A change in salinity regime, by changing predator and parasite abundances and disease incidence, could directly alter adult population fecundity and oyster production; and

(2) A change in bay circulation pattern, by affecting the distribution of oyster larvae, could alter the location of significant brood stock for the bay and affect the success of larval settlement, thereby altering fecundity and production. Because predator and parasite abundances do not change linearly with salinity, because the impact of salinity change on parasite prevalence and infection intensity is more significant in the spring and early summer than at other times, and because the location of brood stock may change, particularly after a major flood, some changes in bay salinity and bay circulation will be more important than others, although the absolute magnitude of change may be similar. And, necessarily, some reefs will be affected more than others within the Galveston Bay system. Consequently, a coupled hydrodynamics-population dynamics model has been developed to assess the potential impact of varying bay salinity and bay circulation to adequately take into account the nonlinearity in biological processes that exists and the interactions among the various oyster populations that certainly do exist in Galveston Bay.

The model consists of the following parts:

1. The hydrodynamics model is a 3-D finite-element circulation model developed by the Waterways Experiment Station, Army Corps of Engineers;

2. The post settlement oyster population dynamics model is an energy flow model tracking oyster growth and fecundity as a function of temperature, salinity, population density, food

supply, turbidity, and water flow. Additional inputs to the oyster component include *Perkinsus marinus* infection intensity, fishing, and predation; and

3. The larval oyster model includes an energy flow model patterned after the post-settlement model and a larval transport model utilizing the hydrodynamics model's flow fields.

The post-settlement component of the oyster model has been used to examine the conditions under which oyster population declines and crashes may occur in bays like Galveston Bay and the importance of seasonal mortality in the population dynamics of the oyster. One of the consistent messages of this modeling exercise is the requirement of mortality for the population to produce larger, market-size individuals. Either adult or juvenile mortality will do, as both juveniles and adults compete for food. Restricting mortality results in crowding, food limitation, and a stunted population. As mortality extends into the juvenile size classes, and finally into the larval stages, the population on the average becomes skewed more and more towards the larger adult size classes. Frequently, but not always, this proportional shift was sufficient to result in a larger number of large adults in absolute terms despite overall lower population densities. An even higher rate of mortality reversed this trend; the population size-frequency shifted again towards smaller size classes as adult individuals were rapidly removed from the population.

Clearly, for a successful fishery, a delicate balance exists between sufficient mortality to permit the fishery to exist and too much mortality, which will reduce the fishable yield. The stability of oyster populations is sensitive to several factors, including the timing and intensity of mortality, latitude, and food supply. Increased mortality reduced population density in every comparison. Oftentimes, a relatively stable equilibrium occurred as recruitment balanced mortality over the long term. In all cases, however, mortality rates sufficient to destabilize this equilibrium could be found and a population decline resulted.

When mortality extended over a wider range of size classes or affected larval survivorship, population destabilization occurred more easily. In the former case, more oysters were exposed to mortality. In the latter case, lowered recruitment no longer balanced the higher rates of mortality. In cases where mortality was imposed for time periods of less than one year, mortality restricted to the six summer months (April-September) nearly always resulted in decreased population density compared to mortality restricted to the winter months. Rarely did the two yield similar results. Never did summer mortality have a lesser impact. The effect was noted at different latitudes, in populations having mortality restricted to a variety of differing size classes, and in populations varying in larval survivorship.

However, adult mortality was required. Extending mortality into the juvenile size classes minimized the effect. Nearly all reports of population crashes in oyster populations result from adult summer mortality, recruitment failure, or floods. Most supply, turbidity, and water flow. Additional inputs to the oyster component include *Perkinsus marinus* infection intensity, fishing, and predation; and

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However, adult mortality was required. Extending mortality into the juvenile size classes minimized the effect. Nearly all reports of population crashes in oyster populations result from adult summer mortality, recruitment failure, or floods. Most predators and parasites are most effective in the summer. Our results suggest that the explanation for the importance of adult summer mortality does not necessarily reside in the fact that the most significant agents of adult mortality (except the fishery) operate most effectively in the summer. Although this may well be true, the oyster itself would appear to be more susceptible to mortality in the summer. That is, a greater chance of population crashes in the summer may be physiologically preordained.

One potentially important mechanism causing this increased susceptibility is the temperature control on the partitioning of somatic tissue and reproductive tissue in the winter, spring, and summer. Fewer individuals are present in the adult size classes in the winter, hence losses are minimized. Juveniles rapidly grow to adulthood in the spring and spawn in the summer. As a result, reproductive effort is higher and population stability is enhanced when mortality is restricted to the winter.

Populations at higher latitudes may be more susceptible to population crashes. Simulated populations in Chesapeake Bay were more susceptible to population crashes than those in Galveston Bay. Simulated populations in Galveston Bay consistently had higher population densities after six years. Reproductive effort was higher because more of the year occurred within the temperature range conducive to spawning. Higher reproductive effort balanced a larger rate of mortality; hence, mortality rates had to be substantially higher in Galveston Bay to effect a population crash. Although not simulated, recovery rates should have been faster as well. Like the distinction between winter and summer mortality, this latitudinal gradient in population stability would appear to originate in the basic physiological milieu of the oyster. The fundamental physiological mechanisms associated with reproduction and the division of net production into somatic and reproductive growth would appear to be responsible. The methods for managing the oyster fishery are generally limited to three somewhat interconnected decisions:

1. what size limit should be set;
2. what season should be allowed; and
3. what population density should trigger season closure?

The setting of size limits may depend on biological and economic issues. Only biological issues will be considered here. Two aspects of oyster physiology are most important in determining size limits.

(1) Under conditions of crowding and at lower latitudes, oysters fail to grow to large size. The former is due to food-limiting conditions. The latter is due to the warmer temperatures shunting net production into reproductive growth. A considerable body of data supports food limitation in oyster populations. A latitudinal gradient in size bespeaks of the importance of temperature and the degree to which net production is allocated to somatic growth. Both phenomena are reproduced by the model. Clearly, in either case, the setting of size limits as currently done has the effect of artificially reducing yield. If economic considerations warrant it, lower size limits should be set in these populations. In crowded conditions, adult mortality might even

increase adult size and yield.

(2) Raising size limits raises population density and, under certain conditions, the resulting increase in reproductive effort can eventually result in an increased number of market-size oysters at the higher size limit.

Such conditions are met in populations of relatively low density where oysters of legal size are already abundant. Of importance is the recognition that this condition only occurs in populations suffering a relatively high degree of mortality relative to the recruitment rate. Many other agents of mortality, besides the fishery, are important in oyster populations and these agents generally do not respect legal size limits. The model suggests that raising size limits will only be effective if the fishery is the predominant cause of mortality in the population or if other agents of mortality are generally restricted to these same size classes. If all adults are affected, then raising size limits will be ineffective. Besides size limits, fishing seasons are typically set. Fishing seasons on public grounds are generally restricted to the winter months. In some cases, certain areas are set aside for a summer season as well. Natural mortality rates are high in oyster populations, generally greater that 70% per year. Oyster populations in the Gulf of Mexico withstand this degree of mortality without long-term population declines.

Rates of recruitment are sufficient to balance mortality over the long term. Nevertheless, population declines do occur and these have, on occasion, been blamed on overfishing. Although no adequate data are available, one suspects that the fishery could be a principle source of mortality in the winter, but not in the summer when the various other agents of mortality, diseases and predators, come into play. Oyster populations are more resistant to winter mortality than summer mortality. The increased likelihood of an intense population decline during the summer observed throughout the oyster's latitudinal range is a product of the basic physiology of the oyster. Simulated oyster populations were most resistant to population declines when mortality was restricted to the winter months under nearly all conditions of recruitment, size-class specific mortality, and food supply: they were never less resistant. The simulations suggest that oyster populations can withstand substantially higher rates of mortality in the winter than in the summer and, under conditions where fishing is the primary cause of mortality, populations should be managed more conservatively during the summer season.

A latitudinal gradient in stability exists in oyster populations. Population declines without short-term recovery are more likely at higher latitudes. The simulations suggest that populations should be more and more sensitive to natural agents of mortality and to management decisions at ever higher latitudes. In effect, populations in the Gulf of Mexico, by their physiology, can withstand the vagaries of nature and the mistakes of man much easier than their brethren on the Mid-Atlantic and northeast coasts of the U.S. This is not accidental. It is inherent to the oyster's physiology and the nature of the population dynamics cycle that accrues therefrom. The evidence suggests the need for a more conservative oyster management at higher latitudes.

In effect, the Gulf of Mexico populations and the northeastern populations exist under different physiological constraints and these constraints demand different, not the same, management philosophies and decisions.